

GPU ACCELERATORS AT JSC

SUPERCOMPUTING INTRODUCTION COURSE

23 May 2024 | Kaveh Haghighi Mood, Andreas Herten | Forschungszentrum Jülich

Outline

GPUs at JSC

JUWELS

JUWELS Cluster

JUWELS Booster

JURECA DC

JUPITER

GPU Architecture

Empirical Motivation

Comparisons

GPU Architecture

Summary

Programming GPUs

Libraries

Directives

CUDA C/C++

Performance Analysis

Advanced Topics

Advanced Topics



JUWELS Cluster – Jülich's Scalable System

- 2500 nodes with Intel Xeon CPUs (2×24 cores)
- 46 + 10 nodes with 4 NVIDIA Tesla V100 cards (16 GB memory)
- 10.4 (CPU) + 1.6 (GPU) PFLOP/s peak performance (Top500: #86)



JUWELS Booster – Scaling Higher!

- 936 nodes with AMD EPYC Rome CPUs (2×24 cores)
- Each with 4 NVIDIA A100 Ampere GPUs (each: $\text{FP64TC: } 19.5$ TFLOP/s, 40 GB memory)
 $\text{FP64: } 9.7$
- InfiniBand DragonFly+ HDR-200 network; 4×200 Gbit/s per node



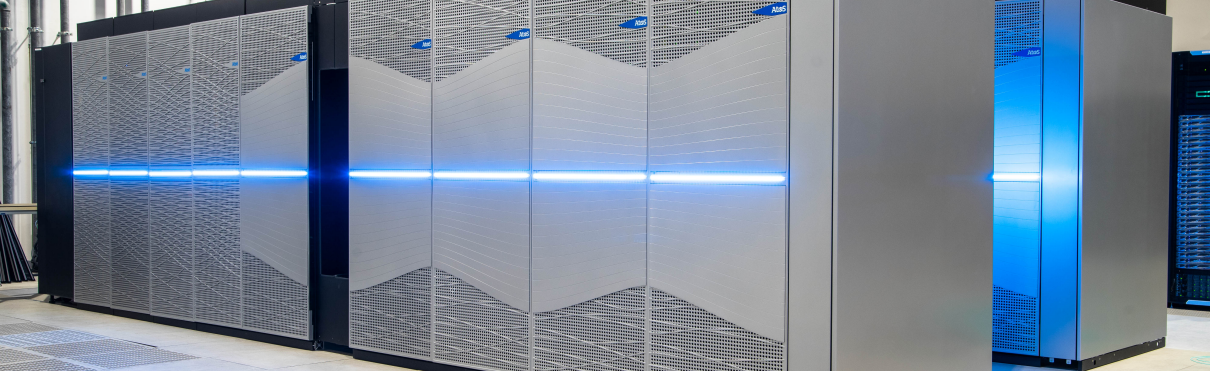
Top500 List Nov 2020:

- #1 Europe
- #7 World
- #4* Top/Green500



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JURECA DC – Multi-Purpose

- 768 nodes with AMD EPYC Rome CPUs (2×64 cores)
- 192 nodes with 4 NVIDIA A100 Ampere GPUs
- InfiniBand DragonFly+ HDR-100 network



JUPITER – Exascale

- First Exascale system in Europe
- Procured by EuroHPC JU, BMBF, MKW-NRW, hosted by JSC
- Currently in pre-installation
- 24 000 NVIDIA H100 GPUs (Grace-Hopper superchips)
- 1 EFLOP/s FP64 (HPL), 32 EFLOP/s FP8 (peak)

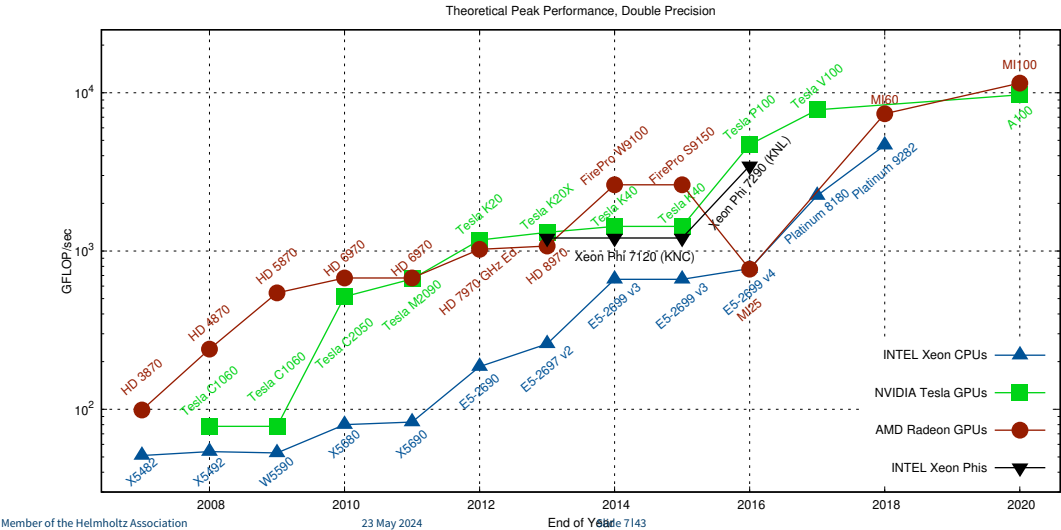
→ jupiter.fz-juelich.de



GPU Architecture

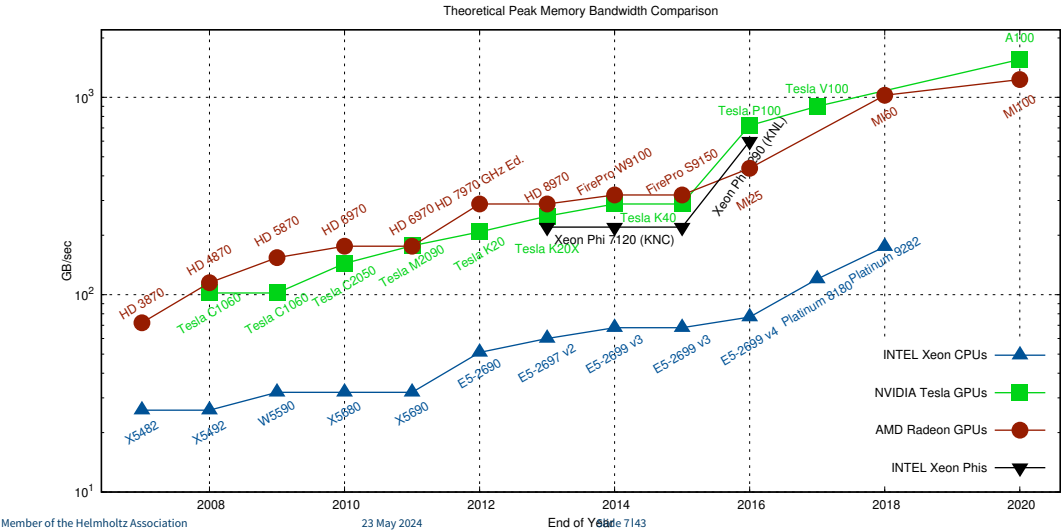
Status Quo Across Architectures

Performance



Status Quo Across Architectures

Memory Bandwidth



CPU vs. GPU

A matter of specialties



CPU vs. GPU

A matter of specialties



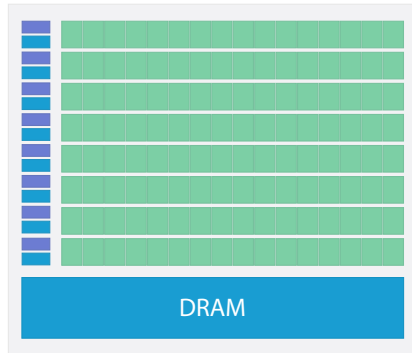
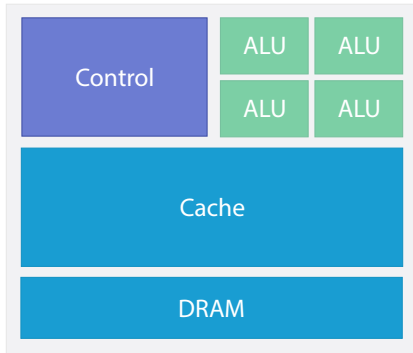
Transporting one



Transporting many

CPU vs. GPU

Chip



GPU Architecture Design

GPU optimized to **hide latency**

- Memory

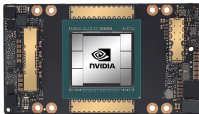
- GPU has small (40 GB), but high-speed memory 1555 GB/s
- Stage data to GPU memory: via PCIe 4 (32 GB/s) or PCIe 5 (64 GB/s) bus
- Stage automatically (*Unified Memory*), or manually

- Two engines: Overlap compute and copy



A100

40 GB RAM, 1555 GB/s

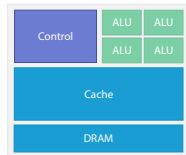


H100

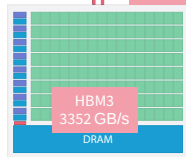
80 GB RAM, 3352 GB/s



Host




PCIe 5
≈64 GB/s



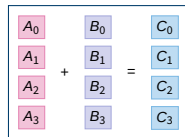
Device

SIMT

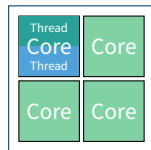
$$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$$

- CPU:
 - Single Instruction, Multiple Data (SIMD)
 - Simultaneous Multithreading (SMT)
- GPU: Single Instruction, Multiple Threads (SIMT)
 - CPU core \cong GPU multiprocessor (SM)
 - Working unit: set of threads (32, a *warp*)
 - Fast switching of threads (large register file)
 - Branching 

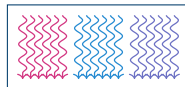
Vector



SMT



SIMT

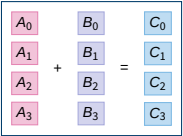


SIMT

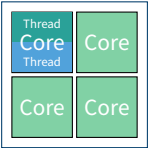
$SIMT = SIMD \oplus SMT$



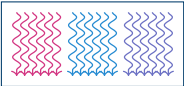
Vector



SMT



SIMT



Graphics: img:amperepictures

SIMT

$SIMT = SIMD \oplus SMT$

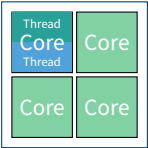


Vector

A_0	B_0	C_0
A_1	B_1	C_1
A_2	B_2	C_2
A_3	B_3	C_3

$+$ $=$

SMT



SIMT



Graphics: img:amperepictures

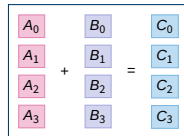
SIMT

$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$

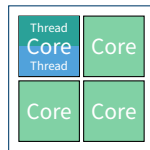
Multiprocessor



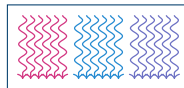
Vector



SMT



SIMT

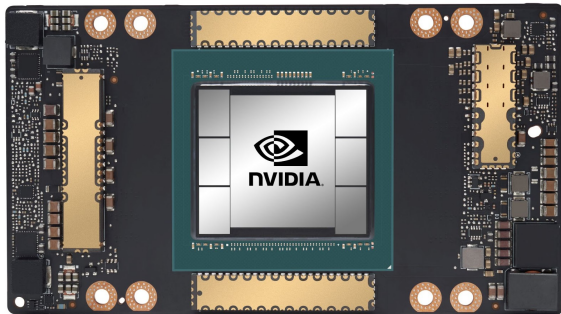


Graphics: img:amp:graphics

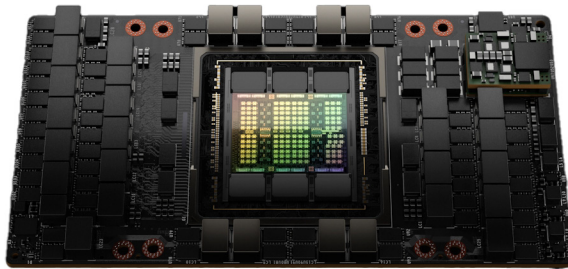
A100 vs H100

Comparison of last vs. current generation

A100



H100



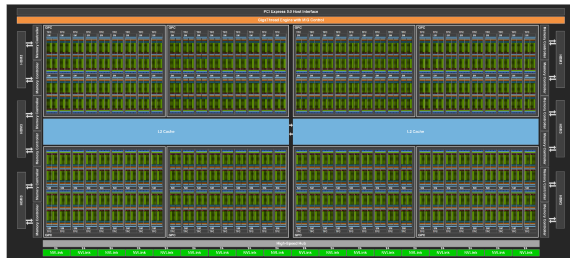
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A100



H100



A100 vs H100

Comparison of last vs. current generation

A100



H100



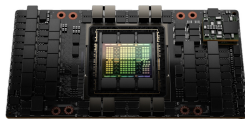
CPU vs. GPU

Let's summarize this!



Optimized for **low latency**

- + Large main memory
- + Fast clock rate
- + Large caches
- + Branch prediction
- + Powerful ALU
- Relatively low memory bandwidth
- Cache misses costly
- Low performance per watt



Optimized for **high throughput**

- + High bandwidth main memory
- + Latency tolerant (parallelism)
- + More compute resources
- + High performance per watt
- Limited memory capacity
- Low per-thread performance
- Extension card

Programming GPUs

Preface: CPU

A simple CPU program!

SAXPY: $\vec{y} = a\vec{x} + \vec{y}$, with single precision

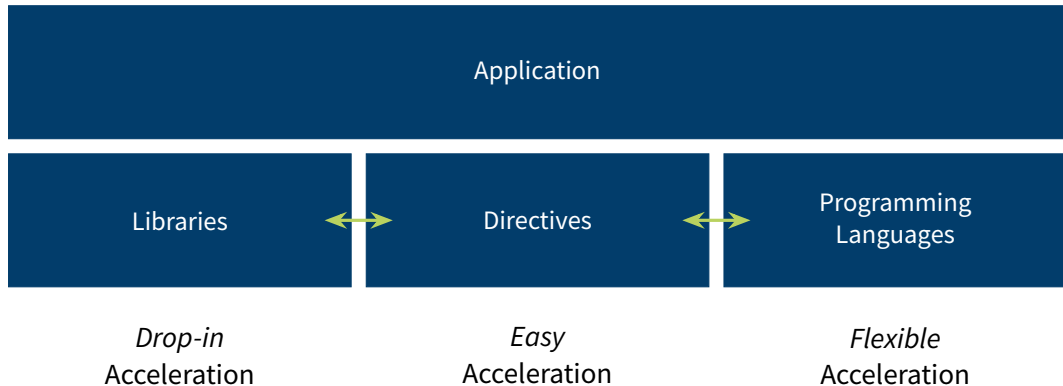
Part of LAPACK BLAS Level 1

```
void saxpy(int n, float a, float * x, float * y) {  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}
```

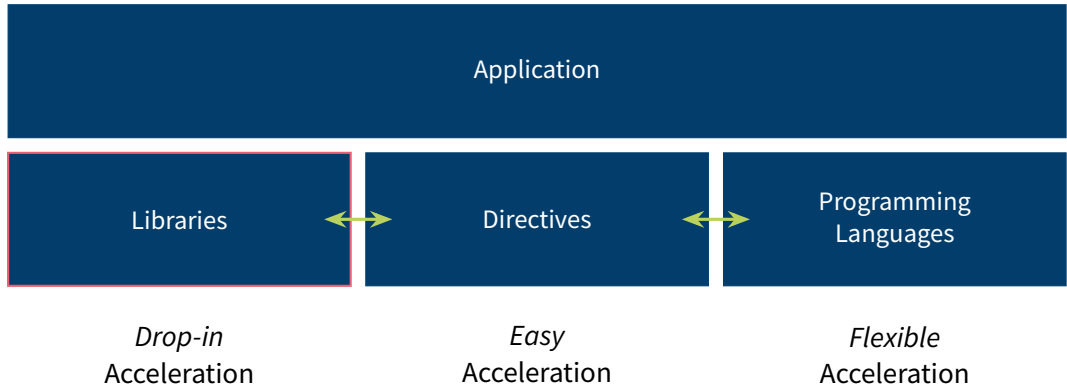
```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
saxpy(n, a, x, y);
```

Summary of Acceleration Possibilities



Summary of Acceleration Possibilities



Libraries

Programming GPUs is easy: Just don't!

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Use applications & libraries

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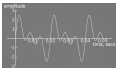
cuBLAS



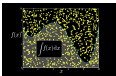
cuSPARSE



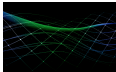
cuDNN



cuFFT



cuRAND



CUDA Math



{A} ARRAYFIRE

Numba

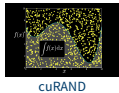
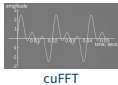


CuPy

Libraries

Programming GPUs is easy: Just don't!

Use applications & libraries



Numba



CuPy



- GPU-parallel BLAS (all 152 routines)
- Single, double, complex data types
- Constant competition with Intel's MKL
- Multi-GPU support

→ <https://developer.nvidia.com/cublas>
<http://docs.nvidia.com/cuda/cublas>

cuBLAS

Code example

```
int a = 42; int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
cublasHandle_t handle;  
cublasCreate(&handle);
```

```
float * d_x, * d_y;  
cudaMallocManaged(&d_x, n * sizeof(x[0]));  
cudaMallocManaged(&d_y, n * sizeof(y[0]));
```

```
cublasSaxpy(handle, n, a, d_x, 1, d_y, 1);
```

```
cublasGetVector(n, sizeof(y[0]), d_y, 1, y, 1);
```

```
cudaFree(d_x); cudaFree(d_y);  
cublasDestroy(handle);
```

cuBLAS

Code example

```
int a = 42; int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
cublasHandle_t handle;  
cublasCreate(&handle);
```

Initialize

```
float * d_x, * d_y;  
cudaMallocManaged(&d_x, n * sizeof(x[0]));  
cudaMallocManaged(&d_y, n * sizeof(y[0]));
```

Allocate GPU memory

```
cublasSaxpy(handle, n, a, d_x, 1, d_y, 1);
```

Call BLAS routine

```
cublasGetVector(n, sizeof(y[0]), d_y, 1, y, 1);
```

Copy result to host

```
cudaFree(d_x); cudaFree(d_y);  
cublasDestroy(handle);
```

Finalize

Programming GPUs

Directives

GPU Programming with Directives

Keepin' you portable

- Annotate serial source code by directives

```
#pragma acc loop
```

```
for (int i = 0; i < 1; i++) {};
```

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- **OpenACC**: Especially for GPUs; **OpenMP**: Has GPU support
- Compiler interprets directives, creates according instructions

GPU Programming with Directives

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- **OpenACC**: Especially for GPUs; **OpenMP**: Has GPU support
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Pro

- Portability
 - Other compiler? No problem! To it, it's a serial program
 - Different target architectures from same code
- Easy to program

Con

- Only few compilers
- Not all the raw power available
- A little harder to debug

OpenACC / OpenMP

Code example

```
void saxpy_acc(int n, float a, float * x, float * y) {  
    #pragma acc kernels  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}  
  
float a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y  
  
saxpy_acc(n, a, x, y);
```

OpenACC / OpenMP

Code example

```
void saxpy_acc(int n, float a, float * x, float * y) {  
    #pragma omp target map(to:x[0:n]) map(tofrom:y[0:n]) loop  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}  
  
float a = 42;  
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Programming GPUs

CUDA C/C++

Programming GPUs Directly

Finally...

Programming GPUs Directly

Finally...

OpenCL Open Computing Language by Khronos Group (Apple, IBM, NVIDIA, ...) 2009

- Platform: Programming language (OpenCL C/C++), API, and compiler
- Targets CPUs, GPUs, FPGAs, and other many-core machines
- Fully open source

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CUDA NVIDIA's GPU platform 2007

- Platform: Drivers, programming language (CUDA C/C++), API, compiler, tools, ...
- Only NVIDIA GPUs
- Compilation with `nvcc` (free, but not open)
`clang` has CUDA support, but CUDA needed for last step
- Also: CUDA Fortran; and more in NVIDIA HPC SDK

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HIP AMD's unified programming model for AMD (via ROCm) and NVIDIA GPUs 2016+

SYCL Intel's unified programming model for CPUs and GPUs (also: DPC++)

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- **Hardest: Come up with parallelized algorithm**

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CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Thread →



CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads →



CUDA's Parallel Model

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- Methods to exploit parallelism:

- Threads → Block



CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Block



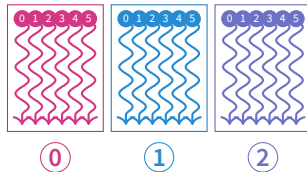
CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks



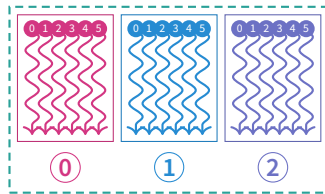
CUDA's Parallel Model

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- Methods to exploit parallelism:

- Threads → Block

- Blocks → Grid



CUDA's Parallel Model

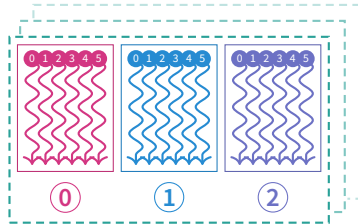
In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks → Grid

- Threads & blocks in 3D



CUDA's Parallel Model

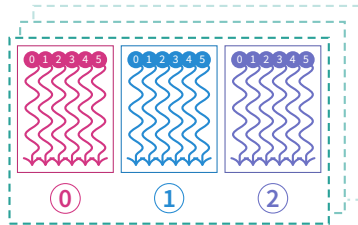
In software: Threads, Blocks

- Methods to exploit parallelism:

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- Blocks → Grid

- Threads & blocks in 3D



- Parallel function: **kernel**

- `__global__ kernel(int a, float * b) { }`
- Access own ID by global variables `threadIdx.x`, `blockIdx.y`, ...

- Execution entity: **threads**

- Lightweight → fast switching!
- 1000s threads execute simultaneously → order non-deterministic!

CUDA SAXPY

With runtime-managed data transfers

```
__global__ void saxpy_cuda(int n, float a, float * x, float * y) {  
    int i = blockIdx.x * blockDim.x + threadIdx.x;  
    if (i < n)  
        y[i] = a * x[i] + y[i];  
}  
  
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y  
cudaMallocManaged(&x, n * sizeof(float));  
cudaMallocManaged(&y, n * sizeof(float));  
  
saxpy_cuda<<<2, 5>>>(n, a, x, y);  
  
cudaDeviceSynchronize();
```

CUDA SAXPY

With runtime-managed data transfers

```
__global__ void saxpy_cuda(int n, float a, float * x, float * y) {  
    int i = blockIdx.x * blockDim.x + threadIdx.x;  
    if (i < n)  
        y[i] = a * x[i] + y[i];  
}
```

Specify kernel

ID variables

Guard against
too many threads

```
int a = 42;  
int n = 10;  
float x[n], y[n];
```

```
// fill x, y
```

```
cudaMallocManaged(&x, n * sizeof(float));
```

```
cudaMallocManaged(&y, n * sizeof(float));
```

Allocate GPU-capable
memory

Call kernel
2 blocks, each 5 threads

```
saxpy_cuda<<<2, 5>>>(n, a, x, y);
```

Wait for
kernel to finish

```
cudaDeviceSynchronize();
```

Programming GPUs

Performance Analysis

GPU Tools

The helpful helpers helping helpless (and others)

■ NVIDIA

`cuda-gdb` GDB-like command line utility for debugging

`compute-sanitizer` Check memory accesses, race conditions, ...

`Nsight` IDE for GPU developing, based on Eclipse (Linux, OS X) or Visual Studio (Windows) or VScode

`Nsight Systems` GPU program profiler with timeline

`Nsight Compute` GPU kernel profiler

■ AMD

`rocProf` Profiler for AMD's ROCm stack

`uProf` Analyzer for AMD's CPUs and GPUs

Nsight Systems

CLI

```
$ nsys profile --stats=true ./poisson2d 10 # (shortened)
```

CUDA API Statistics:

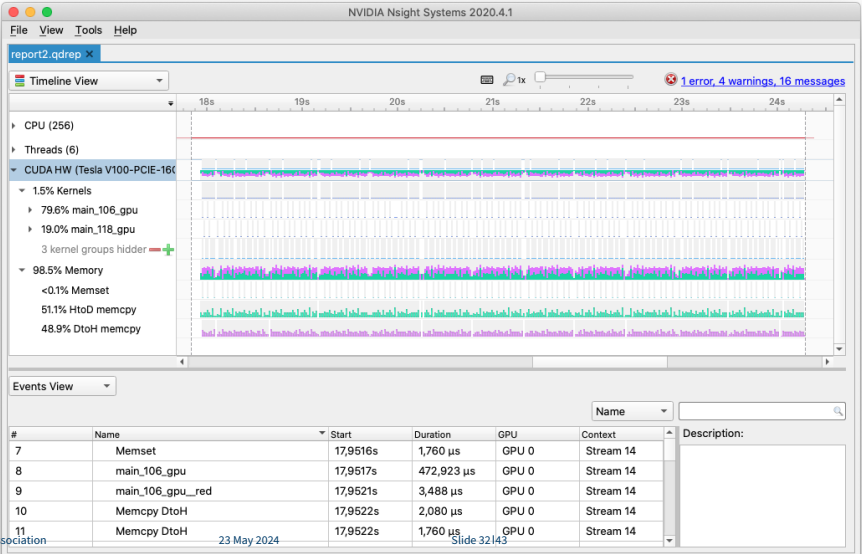
Time(%)	Total Time (ns)	Num Calls	Average	Minimum	Maximum	Name
90.9	160,407,572	30	5,346,919.1	1,780	25,648,117	cuStreamSynchronize

CUDA Kernel Statistics:

Time(%)	Total Time (ns)	Instances	Average	Minimum	Maximum	Name
100.0	158,686,617	10	15,868,661.7	14,525,819	25,652,783	main_106_gpu
0.0	25,120	10	2,512.0	2,304	3,680	main_106_gpu__red

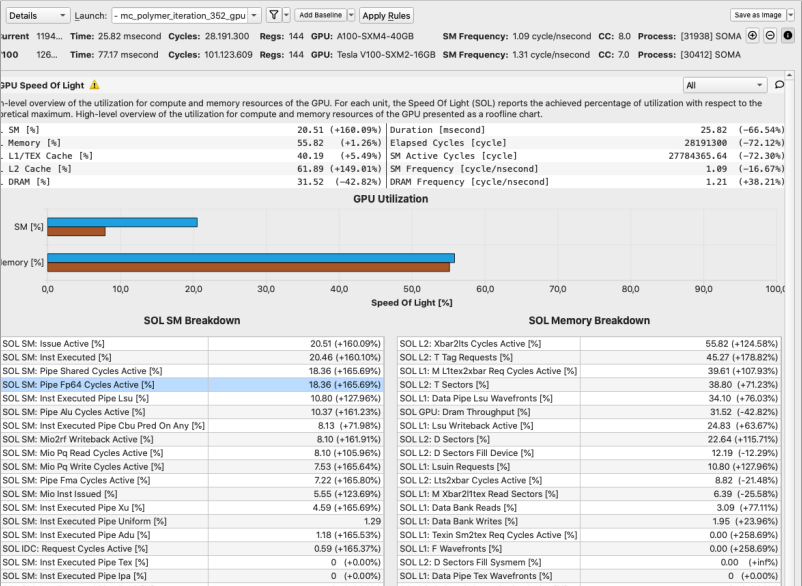
Nsight Systems

GUI



Nsight Compute

GUI



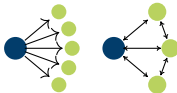
Programming GPUs

Advanced Topics

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So much more interesting things to show!

- Optimize memory transfers to reduce overhead
- Optimize applications for GPU architecture
- Drop-in BLAS acceleration with NVBLAS (`$LD_PRELOAD`)
- Tensor Cores for Deep Learning
- Libraries, Abstractions: [Kokkos](#), [Alpaka](#), [Futhark](#), [HIP](#), [SYCL](#), [C++AMP](#), [C++ pSTL](#), ...
- Use multiple GPUs
 - On one node
 - Across many nodes → MPI
- ...
- Some of that: Addressed at **dedicated training courses**



Using GPUs on JSC Systems

Compiling

CUDA

- Module: `module load CUDA/12`
- Compile: `nvcc file.cu`
- Example cuBLAS: `g++ file.cpp -I$CUDA_HOME/include -L$CUDA_HOME/lib64 -lcublas -lcudart`

OpenACC

- Module: `module load NVHPC/23.7-CUDA-12`
- Compile: `nvc++ -acc=gpu file.cpp`

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MPI CUDA-aware MPIs (with direct Device-Device transfers)

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OpenMPI `module load OpenMPI/4.1.5 MPI-settings/CUDA`

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Containers Use containers via Apptainer (container group needed)

```
$ apptainer pull tf.sif docker://nvcr.io/nvidia/tensorflow:20.12-tf1-py3
```

```
$ srun -n 1 --pty apptainer exec --nv tf.sif python3 myscript.py
```

→ Talk to us at `#cluster-support`

Running

- Dedicated GPU partitions

JURECA DC

`--partition=dc-gpu` 192 nodes

`--partition=dc-gpu-devel` 12 nodes

- Optional

Resource Configuration `--gres=gpu:4`

Account `--account myproject` *or jutil*

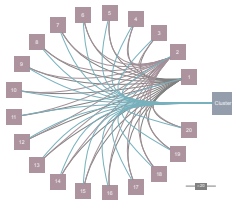
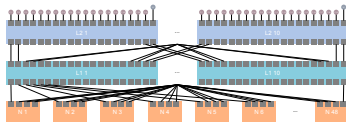
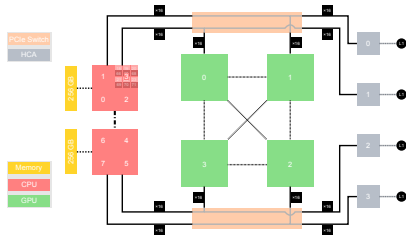
→ See online documentation

Running

JUWELS Booster Topology

- JUWELS Booster: NPS-4 (in total: 8 NUMA Domains)
- Not all have GPU or HCA affinity!
- Network is structured into two levels: In-Cell and Inter-Cell (DragonFly+ network)

→ Documentation: apps.fz-juelich.de/jsc/hps/juwels/



Example

- 16 tasks in total, running on 4 nodes
- Per node: 4 GPUs

```
#!/bin/bash -x
#SBATCH --nodes=4
#SBATCH --ntasks=16
#SBATCH --ntasks-per-node=4
#SBATCH --output=gpu-out.%j
#SBATCH --error=gpu-err.%j
#SBATCH --time=00:15:00
#SBATCH --account=training2310

#SBATCH --partition=dc-gpu
## SBATCH --partition=booster ## JWB
#SBATCH --gres=gpu:4
```

```
srun ./gpu-prog
```

- Submit with `sbatch run.sh`

Reservation

- For days of Hackathon
- Accelerate scheduling through Slurm
- Valid for dc-gpu and booster partition
- Add to batch script / salloc
- `--reservation gpuhack23`

Conclusion

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**Thank you
for your attention!**
a.herten@fz-juelich.de

Appendix

Appendix
Glossary
References

Glossary I

AMD Manufacturer of CPUs and GPUs. 42, 43, 44, 45, 46, 47, 81, 83

Ampere GPU architecture from NVIDIA (announced 2019). 4, 5, 6

API A programmatic interface to software by well-defined functions. Short for application programming interface. 42, 43, 44, 45, 46, 47

CUDA Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 2, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 83

HIP GPU programming model by AMD to target their own and NVIDIA GPUs with one combined language. Short for Heterogeneous-compute Interface for Portability. 42, 43, 44, 45, 46, 47

Glossary II

JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. [2](#), [75](#), [76](#), [77](#), [78](#), [82](#)

JURECA A multi-purpose supercomputer at JSC. [6](#)

JUWELS Jülich's new supercomputer, the successor of JUQUEEN. [3](#), [4](#), [5](#)

MPI The Message Passing Interface, a API definition for multi-node computing. [65](#), [67](#), [68](#), [69](#)

NVIDIA US technology company creating GPUs. [3](#), [4](#), [5](#), [6](#), [16](#), [17](#), [18](#), [42](#), [43](#), [44](#), [45](#), [46](#), [47](#), [60](#), [75](#), [76](#), [77](#), [78](#), [81](#), [83](#)

OpenACC Directive-based programming, primarily for many-core machines. [36](#), [37](#), [38](#), [39](#), [40](#), [67](#), [68](#), [69](#)

Glossary III

- OpenCL** The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 42, 43, 44, 45, 46, 47
- OpenMP** Directive-based programming, primarily for multi-threaded machines. 36, 37, 38, 39, 40
- ROCm** AMD software stack and platform to program AMD GPUs. Short for Radeon Open Compute (*Radeon* is the GPU product line of AMD). 42, 43, 44, 45, 46, 47
- SAXPY** Single-precision $A \times X + Y$. A simple code example of scaling a vector and adding an offset. 24, 57, 58
- Tesla** The GPU product line for general purpose computing computing of NVIDIA. 3

Glossary IV

CPU Central Processing Unit. 3, 6, 11, 12, 13, 15, 16, 17, 18, 24, 42, 43, 44, 45, 46, 47, 81, 83

GPU Graphics Processing Unit. 2, 3, 4, 5, 6, 8, 11, 12, 13, 14, 15, 16, 17, 18, 23, 27, 28, 29, 30, 31, 32, 35, 36, 37, 38, 41, 42, 43, 44, 45, 46, 47, 58, 59, 60, 64, 65, 66, 70, 71, 72, 75, 76, 77, 78, 81, 82, 83

SIMD Single Instruction, Multiple Data. 15, 16, 17, 18

SIMT Single Instruction, Multiple Threads. 14, 15, 16, 17, 18

SM Streaming Multiprocessor. 15, 16, 17, 18

SMT Simultaneous Multithreading. 15, 16, 17, 18

References I

- [2] Karl Rupp. *Pictures: CPU/GPU Performance Comparison*. URL: <https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characteristics-over-time/> (pages 9, 10).
- [6] Wes Breazell. *Picture: Wizard*. URL: <https://thenounproject.com/wes13/collection/its-a-wizards-world/> (pages 27–31).

References: Images, Graphics I

- [1] Forschungszentrum Jülich GmbH (Ralf-Uwe Limbach). *JUWELS Booster*.
- [3] Mark Lee. *Picture: kawasaki ninja*. URL:
<https://www.flickr.com/photos/pochacco20/39030210/> (pages 11, 12).
- [4] Shearings Holidays. *Picture: Shearings coach 636*. URL:
<https://www.flickr.com/photos/shearings/13583388025/> (pages 11, 12).
- [5] Nvidia Corporation. *Pictures: Volta GPU*. *Volta Architecture Whitepaper*. URL:
<https://images.nvidia.com/content/volta-architecture/pdf/Volta-Architecture-Whitepaper-v1.0.pdf>.